# From energy-density functionals to mean field potentials: a systematic derivation

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In this paper we present a systematic method to solve the variational problem of the derivation of a self-consistent Kohn-Sham field from an arbitrary local energy functional. We illustrate this formalism with an application in nuclear physics and give the general mean field associated to the widely used Skyrme effective interaction.

## I. INTRODUCTION

The density functional theory (DFT) is one of the most powerful theories to deal with the intractable quantum many body problem for interacting systems with an arbitrary number of constituents[2]. The original presentation of DFT from the Hohenberg-Kohn theorems[3] establishes an exact mapping between the total ground state energy and the local particle density $\rho(\mathbf{r})$ and has been essentially used in electron structure theory. More general functionals of different local one-body observables can however be used[4, 5]. In particular in nuclear physics, the so called Hartree-Fock formalism with effective density dependent interactions [6, 7, 8] can be seen as one of these extensions.

The practical implementation of density functional theory to electronic or nuclear structure problems is done using self-consistent mean-field Kohn-Sham equations[9]. Within this framework, the interacting problem is reduced to a tractable problem of non-interacting particles moving in an effective potential. The functional form of this effective potential cannot be extracted from the bare interactions, and different approximations are done. A simple local-density approximation (LDA) gives in general poor results, and more involved functionals including gradient terms, kinetic energy densities and spin currents are currently employed[10, 11].

For a given arbitrary functional the definition of the effective mean field potential is formally straightforward from the variational equation $\delta E = \mathrm{tr}\left(\hat{W}\delta\hat{\rho}\right)$. However the actual computation of $\hat{W}$ is tedious and complicated as soon as approximations going beyond LDA are considered. In this article, we present a systematic way to derive the mean field equation or equivalently the self-consistent Kohn-Sham equations when a general functional of any local one-body observable is considered.

## II. MEAN-FIELD FROM DENSITY FUNCTIONAL

Let us consider the most general local energy-density, as a functional of all possible local observables such as densities and currents.

We first introduce the one body density as the observation associated to the one body density operator

$$\rho_{ji} = <\hat{c}_i^+ \hat{c}_j> \tag{1}$$

where $\hat{c}_i^+$ ($\hat{c}_j$) creates (annihilates) a particle in the single particle orbital $|\varphi_i\rangle$. The formalism below can be easily extended to treat paring by introducing the abnormal density $\kappa_{ji} = <\hat{c}_i^+ \hat{c}_j^+>$.

All local observables can be expressed as a function of the one body density as local densities $\rho_{(A,B)}(\mathbf{r})$ defined by the relation :

$$\rho_{(A,B)}(\mathbf{r}) = \mathrm{tr}\left(\delta(\hat{\mathbf{r}} - \mathbf{r})\hat{A}\hat{\rho}\hat{B}\right) \tag{2}$$

where $\hat{\mathbf{r}}$ is the position operator, $\hat{A}$ and $\hat{B}$ are one-body operators characterizing the considered density, and the trace, $tr$, runs over all single particle states. In particular the choice $\hat{A} = \hat{B} = \hat{1}$ leads to the definition of the particle density, while $\hat{A} = \hat{B} = \hat{P}$ gives a kinetic energy density. More examples are worked out in the next section.

According to the most general version of DFT, the local energy density :

$$E = \langle\psi|\hat{H}|\psi\rangle = \int \mathcal{H}(\mathbf{r})\mathrm{d}\mathbf{r} \tag{3}$$

can be expressed as a functional of an ensemble of local densities $\{\rho_{A,B}(\mathbf{r})\}$ associated to an ensemble of operators pairs $(\hat{A}, \hat{B})$ such as:

$$\mathcal{H}(\mathbf{r}) = \mathcal{H}[\rho_{(A,B)}(\mathbf{r})] \tag{4}$$

Using the variational derivation of mean field theory[7], the mean field hamiltonian is defined by the equation

$$\delta E = \mathrm{tr}\left(\hat{W}\delta\hat{\rho}\right) \tag{5}$$

We can thus write the differential of the total energy in

the form :

$$\delta E = \int \delta \mathcal{H}(\mathbf{r}) d\mathbf{r}$$

$$= \sum_{(A,B)} \int \frac{\partial \mathcal{H}}{\partial \rho_{(A,B)}}(\mathbf{r}) \delta \rho_{(A,B)}(\mathbf{r}) d\mathbf{r}$$

$$= \sum_{(A,B)} \int \frac{\partial \mathcal{H}}{\partial \rho_{(A,B)}}(\mathbf{r}) \mathrm{tr}\left(\delta(\hat{\mathbf{r}} - \mathbf{r})\hat{A}\delta\hat{\rho}\hat{B}\right) d\mathbf{r}$$

$$= \mathrm{tr}\left(\sum_{(A,B)} \frac{\partial \mathcal{H}}{\partial \rho_{(A,B)}}(\hat{\mathbf{r}})\hat{A}\delta\hat{\rho}\hat{B}\right) \quad (6)$$

Identifying expression (6) with the mean-field hamiltonian definition (5) we get :

$$\hat{W} = \sum_{(A,B)} \hat{W}_{(A,B)} = \sum_{(A,B)} \hat{B}\frac{\partial \mathcal{H}}{\partial \rho_{(A,B)}}(\hat{\mathbf{r}})\hat{A} \quad (7)$$

### A.  Examples of usual operators

In this part, we will identify the various terms, densities and currents, which are used in the most common density dependent energy functionals with specific local densities $\rho_{(A,B)}(\mathbf{r})$

#### 1.  Particle densities

Let's start with the total particle density $\rho(\mathbf{r})$ that we can write at first :

$$\rho(\mathbf{r}) = \sum_{\alpha} \langle \mathbf{r}, \alpha | \hat{\rho} | \mathbf{r}, \alpha \rangle \quad (8)$$

where the sum over $\alpha$ runs on all additional quantum numbers such as spin and isospin. Introducing the operator $\delta(\mathbf{r} - \hat{\mathbf{r}})$, we can rewrite this expression in a trace form:

$$\rho(\mathbf{r}) = \mathrm{tr}\left(\delta(\mathbf{r} - \hat{\mathbf{r}})\hat{\rho}\right) \quad (9)$$

showing that $\hat{A} = \hat{B} = \hat{1}$ i.e.

$$\rho(\mathbf{r}) = \rho_{(1,1)}(\mathbf{r}) \quad (10)$$

Nuclear functionals generally use spin and isospin densities

$$\rho_{ts}(\mathbf{r}) = \rho_{(\tau_t, \sigma_s)}(\mathbf{r}) \quad (11)$$

where $\hat{\tau}_t$ is the $t$ component of the isospin Pauli operator and $\hat{\sigma}_s$ the $s$ component of the spin Pauli matrix. Of particular importance for asymmetric nuclear matter and exotic nuclei is the isovector particle density

$$\rho_3(\mathbf{r}) = \rho_{(\tau_3, 1)}(\mathbf{r}) \quad (12)$$

where $\hat{\tau}_3$ is the third component of the isospin operator.

Extending the $\hat{\tau}$ and $\hat{\sigma}$ operators to include the identity $\tau_0 = \hat{1}$, and $\hat{\sigma}_0 = \hat{1}$ the definition (11) includes the particle density (10) and the isospin density (12), and can be taken as the most general. Note that since spin and isospin commute the order of the operators $\hat{T}$ and $\hat{\sigma}$ in (11) is not important, $\rho_{ts} = \rho_{st}$. It should also be noticed that, in the nuclear case, the functional is often written in terms of proton and neutron density. In such a case one should use the projector $\hat{\Pi}_n = (\hat{1} + \hat{\tau}_3)/2$ for neutrons and $\hat{\Pi}_p = (\hat{1} - \hat{\tau}_3)/2$ for protons.

#### 2.  Kinetic densities

The case of the kinetic energy density $T(\mathbf{r})$ can be treated in the same way :

$$T(\mathbf{r}) = \sum_{\alpha} \sum_{k} \langle \mathbf{r}, \alpha | \hat{p}_k \hat{\rho} \, \hat{p}_k | \mathbf{r}, \alpha \rangle \quad (13)$$

showing that $T(\mathbf{r})$ is the sum of 3 densities with $(\hat{A}, \hat{B})_k = (\hat{p}_k, \hat{p}_k)$, $k = 1, 3$ i.e.

$$T(\mathbf{r}) = \sum_{k=1,3} \rho_{(p_k, p_k)}(\mathbf{r}) \quad (14)$$

This definition can be extended to introduce spin and isospin as in (11), in particular the isovector kinetic energy density

$$T_3(\mathbf{r}) = \sum_{k=1,3} \rho_{(\tau_3 p_k, p_k)}(\mathbf{r}) \quad (15)$$

More generally the spin and isospin kinetic energy densities can be defined by

$$T_{kts}(\mathbf{r}) = \rho_{(p_k, p_k \tau_t \sigma_s)}(\mathbf{r}) \quad (16)$$

#### 3.  Spin currents

Another important quantity in density functional theory is the spin current $\mathbf{J}(\mathbf{r})$ which is needed to describe the spin-orbit interaction. It is defined by :

$$\mathbf{J}(\mathbf{r}) = -i \sum_{n,\alpha,\alpha'} [\nabla_{\mathbf{r}}\varphi_n(\mathbf{r}, \alpha)] \varphi_n^*(\mathbf{r}, \alpha') \times \langle \alpha' | \sigma | \alpha \rangle + c.c.$$

$$(17)$$

where $\vec{\sigma}$ is the Pauli matrix. Such term can be easily derived from the spin and isospin currents

$$J_{kts}(\mathbf{r}) = \rho_{(p_k, \tau_t \sigma_s)}(\mathbf{r}) + c.c. \quad (18)$$

using $J_i(\mathbf{r}) = \sum_{ks=1}^{3} \varepsilon_{iks} J_{k0s}(\mathbf{r})$, where $\varepsilon$ is the antisymmetric Levi-Cevita tensor.

#### 4. Gradient terms

Energy functional are often written in terms of gradient of densities $\rho_{(A,B)}(\mathbf{r})$. Such terms can also be viewed as (combination of) generalized densities $\rho_{(A',B')}(\mathbf{r})$ using the relation

$$
\begin{aligned}
-i\nabla\,\rho_{(A,B)}(\mathbf{r}) &= \mathrm{tr}\left(\delta(\hat{\mathbf{r}}-\mathbf{r})\left[\hat{\mathbf{p}},\hat{A}\hat{\rho}\hat{B}\right]\right) \\
&= \rho_{(\mathbf{p}A,B)}(\mathbf{r}) - \rho_{(A,B\mathbf{p})}(\mathbf{r}) \qquad (19)
\end{aligned}
$$

Higher order gradients can be similarly expressed if the above expressions are recursively applied:

$$
\begin{aligned}
\vec{\nabla}^n\rho_{(A,B)}(\mathbf{r}) &= (i)^n\sum_{j=0}^{n}(-1)^{n-j}C_n^j\,\cdot \\
&\quad\cdot\;\mathrm{tr}\left(\delta(\hat{\mathbf{r}}-\mathbf{r})\hat{\mathbf{p}}^j\hat{A}\hat{\rho}\hat{B}\hat{\mathbf{p}}^{n-j}\right) \qquad (20) \\
&= \sum_{j=0}^{n}(i)^n(-1)^{n-j}C_n^j\rho_{(\mathbf{p}^jA,B\mathbf{p}^{n-j})}(\mathbf{r})
\end{aligned}
$$

where $C_n^k$ are binomial factors.

### III. APPLICATION TO SKYRME FUNCTIONALS

As a practical application of the above formalism, let us consider the Skyrme nuclear energy-density functional [6, 7, 11] defined by :

$$
\mathcal{H} = \mathcal{K} + \mathcal{H}_0 + \mathcal{H}_3 + \mathcal{H}_{eff} + \mathcal{H}_{fin} + \mathcal{H}_{SO} + \mathcal{H}_{SG} \quad (21)
$$

where the $a_i$ coefficients are linear combination of the usual Skyrme parameters:

$$
\begin{aligned}
\mathcal{K} &= \frac{T}{2m} \\
\mathcal{H}_0 &= a_1\rho^2 + a_2\left(\rho_p^2 + \rho_n^2\right) \\
\mathcal{H}_3 &= \rho^\alpha\left[a_3\rho^2 + a_4\left(\rho_p^2 + \rho_n^2\right)\right] \\
\mathcal{H}_{eff} &= a_5T\rho + a_6\left[T_p\rho_p + T_n\rho_n\right] \\
\mathcal{H}_{fin} &= a_7(\nabla\rho)^2 + a_8\left[(\nabla\rho_p)^2 + (\nabla\rho_n)^2\right] \\
\mathcal{H}_{so} &= a_9\left[\mathbf{J}.\nabla\rho + \mathbf{J}_p.\nabla\rho_p + \mathbf{J}_n.\nabla\rho_n\right] \\
\mathcal{H}_{sg} &= a_{10}\mathbf{J}^2 + a_{11}\left[\mathbf{J}_p^2 + \mathbf{J}_n^2\right]
\end{aligned}
$$

with

$$
\begin{aligned}
a_1 &= \frac{t_0}{4}(2+x_0),\ a_2 = -\frac{t_0}{4}(2x_0+1) \\
a_3 &= \frac{t_3}{24}(2+x_3),\ a_4 = -\frac{t_3}{24}(2x_3+1) \\
a_5 &= \frac{1}{8}\left[t_1(2+x_1) + t_2(2+x_2)\right] \\
a_6 &= \frac{1}{8}\left[t_2(2x_2+1) - t_1(2x_1+1)\right] \\
a_7 &= \frac{1}{32}\left[3t_1(2+x_1) - t_2(2+x_2)\right] \\
a_8 &= -\frac{1}{32}\left[t_2(2x_2+1) + 3t_1(2x_1+1)\right] \\
a_9 &= \frac{W_0}{2},\ \ a_{10} = -\frac{1}{16}(t_1x_1+t_2x_2) \\
a_{11} &= \frac{1}{16}(t_1-t_2)
\end{aligned}
$$

We first write the various terms in terms of generalized densities $\rho_{(A,B)}$

$$
\begin{aligned}
\mathcal{K} &= \frac{\sum_{k=1}^3\rho_{(p_k,p_k)}}{2m} \\
\mathcal{H}_0 &= a_1\rho_{(1,1)}^2 + a_2(\rho_{(\Pi_n,1)}^2 + \rho_{(\Pi_p,1)}^2) \\
\mathcal{H}_3 &= a_3\rho_{(1,1)}^{2+\alpha} + a_4\rho_{(1,1)}^\alpha(\rho_{(\Pi_n,1)}^2 + \rho_{(\Pi_p,1)}^2) \\
\mathcal{H}_{eff} &= a_5\sum_{k=1}^3\rho_{(p_k,p_k)}\rho_{(1,1)} \\
&\quad + a_6(\rho_{(\Pi_n p_k,p_k)}\rho_{(\Pi_n,1)} + \rho_{(\Pi_p p_k,p_k)}\rho_{(\Pi_p,1)}) \\
\mathcal{H}_{fin} &= -a_7\sum_{k=1}^3(\rho_{(p_k,1)} - \rho_{(1,p_k)})^2 \\
&\quad + a_8\left[(\rho_{(p_k,\Pi_n)} - \rho_{(\Pi_n,p_k)})^2 + (\rho_{(p_k,\Pi_p)} - \rho_{(\Pi_p,p_k)})^2\right] \\
\mathcal{H}_{so} &= ia_9\sum_{iks=1}^3\varepsilon_{iks}[\rho_{(p_k,\sigma_s)}.(\rho_{(p_i,1)} - \rho_{(1,p_i)}) \\
&\quad + \rho_{(\Pi_p p_k,\sigma_s)}.(\rho_{(p_i,\Pi_p)} - \rho_{(\Pi_p,p_i)}) \\
&\quad + \rho_{(\Pi_n p_k,\sigma_s)}.(\rho_{(p_i,\Pi_n)} - \rho_{(\Pi_n,p_i)})] \\
\mathcal{H}_{sg} &= a_{10}\sum_{iksk's'=1}^3\varepsilon_{iks}\varepsilon_{ik's'}\rho_{(p_k,\sigma_s)}\rho_{(p_{k'},\sigma_{s'})} \\
&\quad + a_{11}\sum_{iksk's'=1}^3\varepsilon_{iks}\varepsilon_{ik's'}(\rho_{(p_k,\Pi_p\sigma_s)}\rho_{(p_{k'},\Pi_p\sigma_{s'})} \\
&\quad + \rho_{(p_k,\Pi_n\sigma_s)}\rho_{(p_{k'},\Pi_n\sigma_{s'})})
\end{aligned}
$$

Using relation (7), the involved functional derivatives of eq.(5) are reduced to simple derivatives of scalar expressions:

$$W_{\mathcal{K}} = \frac{\hat{\mathbf{p}}^2}{2m}$$

$$W_{\mathcal{H}_0} = 2a_1\rho(\hat{\mathbf{r}}) + 2a_2(\hat{\Pi}_n\rho_n(\hat{\mathbf{r}}) + \hat{\Pi}_p\rho_p(\hat{\mathbf{r}}))$$

$$W_{\mathcal{H}_3} = (2+\alpha)a_3\rho^{1+\alpha}(\hat{\mathbf{r}})$$
$$+ \alpha a_4\rho^{\alpha-1}(\hat{\mathbf{r}})(\rho_n^2(\hat{\mathbf{r}}) + \rho_p^2(\hat{\mathbf{r}}))$$
$$+ 2a_4\rho^{\alpha-1}(\hat{\mathbf{r}})(\hat{\Pi}_n\rho_n(\hat{\mathbf{r}}) + \hat{\Pi}_p\rho_p(\hat{\mathbf{r}}))$$

$$W_{\mathcal{H}_{eff}} = \sum_{k=1}^{3} a_5\hat{p}_k\rho(\hat{\mathbf{r}})\hat{p}_k + a_5T(\hat{\mathbf{r}})$$
$$+ \sum_{k=1}^{3} a_6\hat{\Pi}_n\hat{p}_k\rho_n(\hat{\mathbf{r}})\hat{p}_k + a_6\hat{\Pi}_nT_n(\hat{\mathbf{r}})$$
$$+ \sum_{k=1}^{3} a_6\hat{\Pi}_p\hat{p}_k\rho_p(\hat{\mathbf{r}})\hat{p}_k + a_6\hat{\Pi}_pT_p(\hat{\mathbf{r}})$$

$$W_{\mathcal{H}_{fin}} = -2a_7\Delta\rho(\hat{\mathbf{r}})$$
$$- 2a_8(\hat{\Pi}_n\Delta\rho_n(\hat{\mathbf{r}}) + \hat{\Pi}_p\Delta\rho_p(\hat{\mathbf{r}}))$$

$$W_{\mathcal{H}_{so}} = a_9(\nabla\rho(\hat{\mathbf{r}}) + \nabla\mathbf{J}(\hat{\mathbf{r}})$$
$$+ \hat{\Pi}_n\nabla\rho_n(\hat{\mathbf{r}}) + \hat{\Pi}_n\nabla\mathbf{J}_n(\hat{\mathbf{r}})$$
$$+ \hat{\Pi}_p\nabla\rho_p(\hat{\mathbf{r}}) + \hat{\Pi}_p\nabla\mathbf{J}_p(\hat{\mathbf{r}}))$$

$$W_{\mathcal{H}_{sg}} = 2a_{10}\mathbf{J}(\hat{\mathbf{r}})$$
$$+ 2a_{11}(\hat{\Pi}_n\mathbf{J}_n(\hat{\mathbf{r}}) + \hat{\Pi}_p\mathbf{J}_p(\hat{\mathbf{r}}))$$

The one body mean field operator for the charge $q = n, p$ can be expressed in a more compact form as :

$$\hat{W}_q = \hat{\mathbf{p}}\frac{1}{2m(\hat{\mathbf{r}})}\hat{\mathbf{p}} + U_q(\hat{\mathbf{r}}) + (\hat{\mathbf{p}}\mathbf{V}_q(\hat{\mathbf{r}}) + \mathbf{V}_q(\hat{\mathbf{r}})\hat{\mathbf{p}}) \times \hat{\sigma} \quad (22)$$

where the effective mass is

$$\frac{1}{2m(\hat{\mathbf{r}})} = \left[\frac{1}{2m} + a_5\rho(\hat{\mathbf{r}}) + a_6\rho_q(\hat{\mathbf{r}})\right] \quad (23)$$

while the central potential reads

$$U_q(\hat{\mathbf{r}}) = 2a_1\rho(\hat{\mathbf{r}}) + 2a_2\rho_q(\hat{\mathbf{r}}) + a_3(2+\alpha)\rho^{1+\alpha}(\hat{\mathbf{r}})$$
$$+ a_4\alpha\rho^{\alpha-1}(\hat{\mathbf{r}})(\rho_n^2(\hat{\mathbf{r}}) + \rho_p^2(\hat{\mathbf{r}})) + 2a_4\rho_q(\hat{\mathbf{r}})\rho^\alpha(\hat{\mathbf{r}}) \quad (24)$$
$$+ a_5T(\hat{\mathbf{r}}) + a_6T_q(\hat{\mathbf{r}})$$
$$- 2a_7\Delta\rho(\hat{\mathbf{r}}) - 2a_8\Delta\rho_q(\hat{\mathbf{r}}) + a_9\left(\nabla\mathbf{J}(\hat{\mathbf{r}}) + \nabla\mathbf{J}_q(\hat{\mathbf{r}})\right)$$

and the spin orbit part is given by

$$\mathbf{V}_q(\mathbf{r}) = a_9(\nabla\rho(\hat{\mathbf{r}}) + \nabla\rho_q(\hat{\mathbf{r}})) + 2a_{10}\mathbf{J}(\hat{\mathbf{r}}) + 2a_{11}\mathbf{J}_q(\hat{\mathbf{r}}) \quad (25)$$

consistently with the expressions given in the literature.

## IV. CONCLUSION

In this paper we have introduced a simple and powerful method to solve the variational problem of the derivation of a mean field potential from and arbitrary energy-density functional. Observing that the most general DFT energy functional can be expressed in terms of generalized local one-body densities $\rho_{(A,B)}(\mathbf{r}) = \text{tr}\left(\delta(\hat{\mathbf{r}} - \mathbf{r})\hat{A}\hat{\rho}\hat{B}\right)$, the functional derivative defining the Kohn-Sham or HF field $\hat{W} = \delta E/\delta\hat{\rho}$ can be reduced to the calculation of ordinary derivatives $\partial\mathcal{H}/\partial\rho_{(A,B)}$ of the associated energy density. As an example we have worked out the well known expression of the general Skyrme mean-field. This method gives a simple technique to take into account new terms in future more sophisticated generalized functionals. The autors want to thank M. Bender for the useful discussions.

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